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13. ABSTRACT *(Maximum 200 words)*

A Workshop on "Epitaxy, Interfaces, Defects and Processing of Electronic and Photonic Materials" was held in Pittsburgh, 4-7 November 1991. The following three (3) topic areas were discussed in detail.

(1) Fundamental aspects of two- and three-dimensional epitaxial growth, especially during heteroepitaxy involving misfits, and generation of defects

(2) Atomic structure of interfaces and defects

(3) Growth and processing of electronic and photonic materials using novel concepts

Scientific issues were delineated and approaches or techniques to address these issues were also discussed in detail.

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WORKSHOP

ON

EPITAXY, INTERFACES, DEFECTS AND PROCESSING

OF

ELECTRONIC AND PHOTONIC MATERIALS

DAAL03-91-G-0332

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Final ~~PRELIMINARY~~ REPORT

Since the early eighties, electronic and photonic materials have made great strides. It is now possible to grow very large diameter silicon crystals which are macroscopically dislocation-free. The availability of such crystals has been responsible for the dramatic reduction in fabrication costs of ultra-large-scale integrated circuits.

The demonstration of high temperature superconductivity in cuprate materials has provided impetus for the resurgence of research on novel and exotic superconducting materials. As these materials are extremely brittle, it is a challenge to fabricate them into technologically useful products.

The developments listed above and many other exciting ones are a result of synergistic and interdisciplinary research activities. As the interfacial overlap between different disciplines is enhanced in the future, the importance of such activities will be even more significant.

To further enhance the pace of technological advances, we need to assess *the current status of our understanding of epitaxy, interfaces, defects* and processing of electronic and photonic materials and to delineate areas of future research and development in these materials. The resolution of these issues is central to on our industrial competitiveness.

The preliminary report has been organized as follows. First, significant research accomplishments are highlighted, followed by a brief discussion of enabling technologies. Second, the current status is assessed. Third, critical research areas and directions are emphasized. Fourth, potential scientific and technological benefits are delineated.

• Recent Research Highlights

The developments in electronic and photonic materials over the last ten years have been very impressive. As a result, the technology base has been advanced substantially.

The following constitutes significant developments over the last five years:

(i) Surface emitting microlaser arrays.

(ii) Quantum wire and quantum dot structures.

(iii) High-speed epitaxial devices.

(iv) Blue-light emitting devices.

The fabrication of microlaser arrays required significant developments in synthesis and processing of materials. These structures would not have been possible without our ability to deposit extremely thin epitaxial layers of different compositions, to monitor and characterize their growth in situ and to process structures at nanolevel.

The growth of quantum wire and quantum dot structures depended also on our ability to fabricate nanostructures and to grow epitaxial layers in a controlled manner. Both MBE and OMVPE have been used to grow such structures.

The development of high speed epitaxial devices, such as MODFET's and blue-light emitting lasers, would not have been possible without our ability to dope III-V and II-VI materials in a controlled manner. Furthermore, the fabrication of heterojunction bipolar transistors involving silicon and silicon-germanium layers depended critically on our ability to grow these layers at low temperatures.

• Current Status

(i) Synthesis and Processing - Over the last decade, we have made considerable progress in synthesis and processing. Superlattice and quantum well structures having controlled layer thickness, interface abruptness and composition homogeneity can be grown. In situ growth monitoring techniques have facilitated this. Recently, the application of "Reflection Difference Spectroscopy" to monitor OMVPE growth has clarified the layer growth mechanism. Also, doping can be controlled at a monolayer level (δ-doping).

The availability of sophisticated growth techniques has permitted epitaxial integration of dissimilar materials. For example, semiconductor/metal/semiconductor, semiconductor/insulator/semiconductor and superconductor/insulator/metal multi-layer structures have been grown successfully.

By manipulating the step structure of surfaces of non-polar semiconductors, polar semiconductors free from inversion domain boundaries have been overgrown. In systems involving large misfits, the defect density in the overgrowth is very high. As a result, the overgrowths are not suitable for the fabrication of minority carrier devices.

In situ processing of device structures is being explored. The patterning of substrates using focussed ion beams and subsequent overgrowth in patterned regions have been demonstrated.

(ii) Materials Characterization - Information on structure and composition of surfaces and interfaces can be obtained using STM and Z-contrast microscopy. The latter can be complemented by HREM analysis of interfaces. The first two techniques provide direct images and can thus discover unanticipated effects, whereas the interpretation of HREM images requires a structure model with

image simulation. Ion beams and X-rays can also be used to accurately evaluate the average structure and roughness of interfaces, and modeling is also required for obtaining detailed structural information.

The ballistic electron emission microscopy can provide information on local electronic properties of interfaces. It is also possible to evaluate electronic properties of interfaces and interface defects using electron energy loss spectroscopy. In addition, photoluminescence (PL) and transport measurements can be used to assess optical and electronic properties.

Currently, it is difficult to correlate the structural and composition information generated by Z-contrast imaging and HREM with optical and electronic properties ascertained by PL and transport measurements. This difficulty stems from the lack of reliable model interfaces and the fact that the length scales involved in the two sets of measurements may be considerably different.

(iii) Theory and Simulation - The prediction of structural stability from quantum mechanical total energy calculations is now possible. This technique has been applied to understand observed surface and interface structures, defects, dynamical properties (diffusion) and stability of different phases. In addition, accurate description of electronic and optical properties for idealized systems has been obtained.

The simulations involving empirical interactions have helped us to rationalize the role of surface reconstruction in atomic ordering, dislocation core structures and structures of grain boundaries. Also, the flow patterns in OMVPE reactors have been successfully modelled.

• Major Unresolved Issues

The development of nano-electronics would require thinner layers and sharper interfaces, both in the vertical and lateral directions. To fully exploit

the diversity in properties of available materials, the preceding objective is not limited to elemental and binary materials, but also must include ternary and quaternary III-V and II-VI materials. The difficulty with these materials is that the composition inhomogeneities exist at a scale of 10 nm.

The following are key issues that need to be resolved to achieve the above objective:

(i) <u>Understanding and identifying key atomic processes responsible for initial stages of growth</u> - Our ultimate goal is to understand the synthesis of an interface during epitaxial growth. We believe this can be achieved by assessing and understanding the roles of surface diffusion, steps and surface reconstruction and surfactants in the initiation of growth, island coalescence, mechanisms of dopant incorporation, and 2D to 3D transition. Also, we must discern how these processes are affected by patterning of underlying substrates.

(ii) <u>Understanding and identifying key atomic processes responsible for strain accommodation and defect motion</u> - To grow epitaxial structures involving dissimilar materials that have technological applications, we must understand how threading and misfit dislocations are introduced in the overgrowth when (a) the substrate is macroscopically dislocation-free and the crystal structures of the substrate and the overgrowth are the same and (b) the substrate is dislocated and the crystal structures of the substrate and the overgrowth are the same. Two additional situations develop if one assumes that the crystal structure of the overgrowth is different from that of the substrate.

(iii) <u>Influence of "microstructures" on electronic and optical properties</u> - The term "microstructure" encompasses interface roughness (composition and structure), phase separation, atomic ordering and lateral inhomogeneities. We

need to understand how interface roughness is affected by phase separation, and how the above "microstructural" features influence electronic and optical properties.

(iv) Other Issues - We currently do not understand the chemistry of substractive reactions occurring during reactive ion etching. Also, the formulation of Schottky and ohmic contacts for compound semiconductors is totally empirical. We need to develop generic ideas for these purposes. We should also examine the integration of magnetic and semiconducting materials.

- **Plausible Approaches**

To address the unresolved issues outlined above, we have to develop an integrated approach encompassing synthesis and processing, characterization and modeling. This is of paramount importance as the dimensions of the structures are reduced to nano-level.

We need to establish the usefulness of STM in determining local composition. To achieve this, simulation as well as first-principles theory are required. We also need to explore the effectiveness of STM in studying interfaces. Enhancing the resolution of TEM techniques to the level of 0.1nm, coupled with quantitive interpretation of images and energy loss spectra, would go a long way in addressing the issues of structural and chemical sharpness of interfaces.

Both experimental and theoretical work should be carried out to understand the step structure of III-V surfaces; STM appears to be a logical choice for these experimental studies.

To gain a better understanding of the electronic properties of interfaces, we need to study model metal-semiconductor systems using BEEM.

An attempt should be made to correlate the electronic properties of the interface with its structure.

The systematics of the introduction of dislocations during the growth of heteroepitaxial structures needs to be established. Appropriate growth experiments, together with detailed characterization by TEM and theory, should provide the answer. We also need to discern the effects of dislocations and stacking faults on the electronic properties of III-V semiconductors.

- **Potential Benefits**

In general, a deeper understanding of underlying science of advanced materials would lead to novel materials having unique and exotic properties which may have ramifications in leading-edge technologies. Specifically, we anticipate the following benefits: (i) development of human resources, (ii) integration of diverse materials and devices, (iii) 3D integration of devices using controlled growth, (iv) reliable, fast, efficient, small and cheaper electronic devices, and (v) enhanced industrial competitiveness.